ARKIV FÖR FYSIK Band 13 nr 14

Communicated 13 November 1957 by Oskar Klein and Ivar Waller

Approach to the quantum mechanical many-body problem with strong two-particle interaction I

By Evert Andersén and Ulf Uhlhorn

With 1 figure in the text

Introduction

The methods which are discussed in the following paper have been developed with the nuclear many-body problem, formulated as a classical quantum mechanical many-body problem with only two-particle interaction and without any assumption of the origin of nuclear forces, in mind. The success of the shell model has created the very simple picture of the nucleus according to which a nucleon moving through the nuclear matter is acted upon by a force from all the other nucleons, represented by an average potential. On the other hand the shortness of the range of internucleon forces implies that one nucleon is interacting strongly with a very limited number of other nucleons at a time.

Considerations of this kind have led people to different approaches to the many-body problem. Brueckner and collaborators [1] starting from formal scattering theory have developed a formalism which in a direct way takes account of strong two-particle interactions of short range in large systems. However, as pointed out by Hugenholtz [2] the method of Brueckner is in essence an approximation method for the imperfect Fermi gas, and its applicability to a real nucleus of finite size and high density is questionable. The many-body problem with hard sphere interaction has been treated by several authors [3] but their main interest has not been in the nuclear many-body problem.

From the arguments given above it seems plausible that it is advantageous to use two-particle orbitals in the description of the entire many-particle system. We have tried to develop a consistent mathematical procedure for such a description. Our starting point is a variational method for the solution of the n-particle Schrödinger equation. Two approaches characterized by different n-particle trial wave functions are discussed and the general equations for the determination of (in a certain sense) "best two-particle orbitals" are derived. Both methods may be regarded as extensions of the Hartree–Fock method. The general equations derived, though in principle simple, have a somewhat complicated appearance when written out explicitly, and other approximate methods are therefore examined.

For this purpose it is of interest to examine the problem of two interacting particles in a common potential. It is very convenient to choose this common potential as an oscillator, because then the Hamiltonian will be separable if center of mass and relative coordinates are introduced. Also more physical arguments favour the choice of the oscillator potential (See appendices 1 and 2).

Discussion of trial wave functions

We shall assume that the Hamiltonian **H** of the n-particle system considered contains only two-particle interaction derived from a potential $\mathbf{v}$, which is strong and has a short range:

$$\mathbf{H} = \sum_1^n \mathbf{h}_i + 1/2 \sum_1^n \sum_1^n \mathbf{v}_{ij}. \tag{1}$$

Here **h** is the sum of kinetic and potential energy for one particle. Let z be any number. It is convenient to write $\mathbf{H} - z\mathbf{1}$ as a sum of two-particle operators

$$\mathbf{H} - z\mathbf{1} = \sum_{i<j}\sum \mathbf{0}_{ij}(z), \tag{2}$$

where thus

$$\mathbf{0}_{ij}(z) = (\mathbf{h}_i + \mathbf{h}_j)/(n-1) - 2z\mathbf{1}/(n-1)\,n + \mathbf{v}_{ij}. \tag{3}$$

Let x be a complete set of commuting observables for one particle and denote by

$$\langle x_1', \ldots, x_n' \,|\, E \rangle \tag{4}$$

the corresponding representative of the normalized eigenvector $|E\rangle$ of (1) belonging to the eigenvalue E of **H**.

The usual procedure is to approximate (4) by products of one-particle functions (symmetrized or antisymmetrized)

$$\langle x_1', \ldots, x_n' \,|\, E \rangle \sim \prod_{i=1}^n f_i(x_i'). \tag{5}$$

The effect of the interaction is considered as a perturbation on the one-particle orbitals. The only dependence between two particles which is introduced is that resulting from the symmetry requirements. In problems involving strong interaction this procedure fails because the dependence between two particles will be strong, though possibly sometimes of limited range. In general perturbation theory will not be able to take account of these "correlation" effects. This is very clearly illustrated by the problem of two particles interacting strongly in a common potential (Appendices 1, 2).

It is thus necessary to include the effect of the strong interaction in the form of the approximate wave function. This should be done in such a way that the approximate wave function is exact in the case $n = 2$. It seems natural to divide up the n-particle system in disjoint pairs (and one single particle if n is odd) and write the approximate wave function as a (symmetrized or antisymmetrized) product

$$\begin{aligned} &\langle x_1', \ldots, x_n' \,|\, E \rangle \sim \varphi_1(x_1', x_2')\,\varphi_2(x_3', x_4') \ldots \varphi_{\frac{n}{2}}(x_{n-1}', x_n') \ (n \text{ even}), \\ &\langle x_1', \ldots, x_n' \,|\, E \rangle \sim \varphi_1(x_1', x_2') \ldots \varphi_{\frac{n-1}{2}}(x_{n-2}', x_{n-1}')\,\varphi(x_n) \ (n \text{ odd}). \end{aligned} \tag{6}$$

The two-particle functions $\varphi_i(x', x'')$ are assumed to have the correct symmetry. As a first approximation they may e.g. be taken as the eigen functions of some definite two-particle Hamiltonian

$$\alpha(\mathbf{h}_1 + \mathbf{h}_2) + \beta \mathbf{v}_{12} \tag{7}$$

with numerical coefficients α and β.

The trial function (6) is by far not the only one containing two-particle dependence. One of the simplest choices is the following

$$\langle x_1', \ldots, x_n' \,|\, E\rangle \sim \prod_{i<j} f(x_i', x_j') \quad (1 \leqslant i < j \leqslant n) \tag{8}$$

where the product is over all possible $n(n-1)/2$ pairs and the two-particle function $f(x', x'')$ is symmetric or antisymmetric. The correct symmetry of the whole product is then automatically guaranteed. This is obvious in the symmetric case. In the antisymmetric case consider the interchange of particles i and $i+1$. The only change occurs in the factor $f(x_i', x_{i+1}')$ the sign of which is reversed. As any permutation may be built up from transpositions of neighbouring elements the statement is proved. At first sight the trial function (8) seems to be very restricted as it contains only one two-particle function. That this restriction is not serious will be shown by an example.

We shall refer to (6) as the disjoint pair function and to (8) as the overlapping pair function.

The variational procedure

The eigenvalue problem

$$\mathbf{H}\,|\,E\rangle = E\,|\,E\rangle \tag{9}$$

is equivalent to the variational problem

$$\text{to find the extremum of } \langle E\,|\mathbf{H}|\,E\rangle - E\,(\langle E\,|\,E\rangle - 1) \ \text{ over } |\,E\rangle \text{ and } E. \tag{10}$$

Disjoint pair function. In the variational problem we replace $|\,E\rangle$ by the expression (6). The variations of the functions $\varphi_m(x_i, x_j)$ are considered as independent and subject to no subsidiary condition beside the requirement of correct symmetry. (The procedure is thus different e.g. from the usual way of deriving Fock's equations where orthonormality of the one-particle trial wave functions is prescribed.) The expression to be varied is now with selfevident notations

$$\langle {}^{1}_{12} | \langle {}^{2}_{34} | \ldots \sum_{i<j}\sum \mathbf{0}_{ij}(E)\,\mathbf{S}\,|\, {}^{1}_{12}\rangle \ldots |\, {}^{n/2}_{n-1,n}\rangle \quad (n \text{ even}) \tag{11}$$

where $\mathbf{S}$ is an operator giving correct symmetry to the ket to the right of it. We note that $\sum_{i<j}\sum \mathbf{0}_{ij}(E)$ is a symmetric operator and thus commutes with $\mathbf{S}$. Variation of the two-particle orbital $|{}^{1}\rangle$ gives the equation

$$\langle {}^{2}_{34} | \ldots \langle {}^{n/2}_{n-1,n} | \sum_{i<j}\sum \mathbf{0}_{ij}(E)\,\mathbf{S}\,|\, {}^{1}_{12}\rangle \ldots |\, {}^{n/2}_{n-1,n}\rangle = 0 \quad (n \text{ even}). \tag{12}$$

One such equation is obtained for every two-particle orbital. These equations are all linear in one orbital and bilinear in all the others. The case with n odd is treated completely analogously.

The equations obtained above correspond to Fock's equations obtained by an analogous one-particle orbit method. The expression to be varied in that case is

$$\langle \genfrac{}{}{0pt}{}{1}{1} | \langle \genfrac{}{}{0pt}{}{2}{2} | \dots \langle \genfrac{}{}{0pt}{}{n}{n} | \sum_{i<j}\sum \mathbf{0}_{ij}(E)\, \mathbf{S} \, | \genfrac{}{}{0pt}{}{1}{1} \rangle \dots | \genfrac{}{}{0pt}{}{n}{n} \rangle, \tag{13}$$

and the equations obtained

$$\langle \genfrac{}{}{0pt}{}{2}{2} | \dots \langle \genfrac{}{}{0pt}{}{n}{n} | \sum_{i<j}\sum \mathbf{0}_{ij}(E)\, \mathbf{S} \, | \genfrac{}{}{0pt}{}{1}{1} \rangle \dots | \genfrac{}{}{0pt}{}{n}{n} \rangle = 0. \tag{14}$$

By a linear transformation in the n-dimensional space of the one-particle orbits the equations (14) are brought on the customary form (orthonormalization) and this transformation does not affect the normalized state vector of the whole system

$$\sum_{j=1}^{n} \langle \genfrac{}{}{0pt}{}{j}{2} | \mathbf{0}_{12}(0) \{ | \genfrac{}{}{0pt}{}{i}{1} \rangle | \genfrac{}{}{0pt}{}{j}{2} \rangle - | \genfrac{}{}{0pt}{}{j}{1} \rangle | \genfrac{}{}{0pt}{}{i}{2} \rangle \} = \epsilon_i | \genfrac{}{}{0pt}{}{i}{1} \rangle. \tag{15}$$

Returning to our equations (12) we note that it is possible to choose here the two-particle orbits orthonormalized. It is, however, questionable if a further linear transformation of the orbits would in general lead to simpler equations. In principle it is possible to determine the set of solutions to the equations by an iterative process analogue to Hartree's method. However, already in the case of few particles this will be very laborious and it is necessary to choose other simpler methods.

Overlapping pair function. In the variational problem (10) we replace $| E \rangle$ by the expression (8). The expression to be varied is now

$$\iiiint d\,(x_i' \, x_j' \, x_i'' \, x_j'') \{ \prod_{i<j} f\,(x_i', x_j') \} \{ \sum_{i<j}\sum \langle x_i', x_j' | \mathbf{0}\,(E) | x_i'', x_j'' \rangle \} \{ \prod_{i<j} f\,(x_i'' \, x_j'') \}. \tag{16}$$

The two-particle function $f\,(x_i', x_j')$ is varied without any other subsidiary condition than the requirement of correct symmetry. The equation for the determination of $f\,(x_i, x_j)$ is essentially nonlinear.

Simplified methods

The equations obtained from the variational procedure are even for a small number of particles so complicated that an exact solution would be extremely laborious. As the interaction is strong it is doubtful if a perturbation method or an iterative procedure is suitable. For simplification we restrict the admitted two-particle orbitals in the variational procedure. The first step in this simplification is to choose only two-particle wave functions which can be written as products of functions depending respectively on the sum and the difference of the space-coordinates of two particles (in the following x denotes the three-dimensional position vector of one particle):

$$f_m\,(x_1', x_2') = s_m \left(\frac{x_1' + x_2'}{\sqrt{2}} \right) d_m \left(\frac{x_1' - x_2'}{\sqrt{2}} \right). \tag{17}$$

In the symmetric case $d_m\,(z)$ must be an even function, in the antisymmetric case $d_m\,(z)$ must be an odd function. The $d_m\,(z)$:s and $s_m\,(z)$:s must not necessarily be all different. E.g. we can choose all the $d_m\,(z)$:s equal.

In order to simplify the equation we choose for $s_m(z)$ and $d_m(z)$ suitable functions depending on a small number of parameters. The functions $s_m(z)$ are required to have the property that for certain values of the parameters the wave function of the whole system describes noninteracting particles in a common potential. The deviation of the parameter values from these "shell model" values thus describes the "correlation" effect of the interaction. To fulfill these requirements we take for $f_m(x_1', x_2')$ eigen solutions of the problem of two interacting particles in a common oscillator potential. The requirement of separability uniquely determines the common potential as an oscillator. The constants of the corresponding Hamiltonian are chosen as variational parameters. If the interaction is taken to be a square well the two-particle wave functions may be written as closed expressions involving Whittaker's functions (See appendix 1). For a first preliminary discussion we choose both $d_m(z)$ and $s_m(z)$ as oscillator wave functions but with different parameters.

Discussion of trial wave functions for one-dimensional systems

In order to investigate the consequences of the discussion given above we consider the simplest possible example, a system of one-dimensional interacting particles, with coordinates $x_1, \ldots, x_n$. Our trial wave functions are chosen of the form

$$\varphi_m(x_1, x_2) = H_{m\oplus}((2\sqrt{k_\oplus}(x_1+x_2))\cdot$$
$$H_{m\ominus}((2\sqrt{k_\ominus}(x_1-x_2))\exp\{-k_\oplus(x_1+x_2)^2-k_\ominus(x_1-x_2)^2\} \quad (18)$$

where $H_{m\oplus}(z)$ and $H_{m\ominus}(z)$ are Hermite polynomials. $H_{m\ominus}(z)$ is even or odd depending on the required symmetry or antisymmetry of $\varphi_m(x_1, x_2)$. If $k_\oplus = k_\ominus$, $\varphi_m(x_1, x_2)$ is a wave function for two noninteracting particles in a common oscillator potential.

Disjoint pair trial function. For the ground state of a system of bosons we take $m_\oplus = m_\ominus = 0$

$$\begin{aligned}\varphi(x_1, x_2) &= \exp\{-k_\oplus(x_1+x_2)^2-k_\ominus(x_1-x_2)^2\},\\ \Psi(x_1, \ldots, x_n) &= N\exp\{-k_\oplus\sum_{i<j}\sum(x_i+x_j)-k_\ominus\sum_{i<j}\sum(x_i-x_j)^2\}.\end{aligned} \quad (19)$$

For the ground state of a system of fermions (even number n of particles) we take $m_\oplus + m_\ominus = 4m-3$ $(m = 1, \ldots, n/2)$ and $m_\ominus$ odd. If $k_\oplus - k_\ominus = 0$ the wave function is

$$\Psi(x_1 \ldots x_n) = N\exp\{-(k_\oplus + k_\ominus)\sum_{i=1}^{n} x_i^2\}\begin{vmatrix} H_0(x_1) \ldots H_{n-1}(x_1)\\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot\ \cdot \\ H_0(x_n) \ldots H_{n-1}(x_n)\end{vmatrix} \quad (20)$$

(See appendix 3). As was required this wave function describes n noninteracting particles in a common oscillator potential.

Overlapping pair trial function. For the ground state of a system of bosons the wave function is the same as in the previous case (19). For the ground state of a system of fermions we take $m_\oplus = 0$, $m_\ominus = 1$ i.e.

$$f(x_1, x_2) = (x_1 - x_2)\exp\{-k_\oplus(x_1+x_2)^2-k_\ominus(x_1-x_2)^2\}. \quad (21)$$

In appendix 3, it is shown that

$$\prod_{1\le i<j\le n}(x_i-x_j)=\begin{vmatrix} H_0(x_1)\ldots H_{n-1}(x_1)\\ \cdot\;\cdot\;\cdot\;\cdot\;\cdot\;\cdot\;\cdot\;\cdot\;\cdot\\ H_0(x_n)\ldots H_{n-1}(x_n)\end{vmatrix}. \tag{22}$$

The total wave function is then

$$\Psi(x_1\ldots x_n)=N\prod_{1\le i<j\le n} f(x_i,x_j)=$$

$$=N\exp\{-(n-1)(k_\oplus+k_\ominus)\sum_{i=1}^{n}x_i^2-(k_\oplus-k_\ominus)\sum_{i=j}\sum x_i x_j\}\begin{vmatrix} H_0(x_1)\ldots H_{n-1}(x_1)\\ \cdot\;\cdot\;\cdot\;\cdot\;\cdot\;\cdot\;\cdot\;\cdot\\ H_0(x_n)\ldots H_{n-1}(x_n)\end{vmatrix}. \tag{23}$$

If $k_\oplus=k_\ominus$ this is just the wave function (20) describing noninteracting particles.

It should be remarked that the discussion given above is independent of the form of the polynomials. It is possible to choose instead of Hermite polynomials simple powers or any other set of polynomials of the same degree.

Determination of the ground state of a system of bosons. As indicated above the trial wave function is given by (19). In order to make the calculations simple we assume that the interaction between the particles is derived from a Gauszian potential $V_0\exp-\beta(x_i-x_j)^2$ and that the common potential is an oscillator. The Hamiltonian of the system is then

$$\mathbf{H}=-\frac{\hbar^2}{2m}\sum_i\frac{\partial^2}{\partial x_i^2}+\frac{m}{2}\omega^2\sum_i x_i^2+\frac{1}{2}V_0\sum_{i\neq j}\sum e^{-\beta(x_i-x_j)^2}. \tag{24}$$

We write the wave function as

$$\Psi(x_1,\ldots,x_n)=N e^{-\frac{K}{4}\Sigma x_i^2-\frac{k}{4}\sum_{i\neq j}\Sigma x_i x_j} \tag{25}$$

where

$$K=4(n-1)(k_\oplus+k_\ominus) \text{ and } k=4(k_\oplus-k_\ominus).$$

By elementary integrations the expected value of the Hamiltonian (24) is determined as a function of k and K:

$$\begin{aligned}\langle\mathbf{H}\rangle&=T+V_{\text{pot}}+V_{\text{int}},\\ T&=\frac{\hbar^2}{2m}\frac{1}{4}nK\\ V_{\text{pot}}&=\frac{1}{4}m\omega^2\frac{n(K+(n-2)k)}{(K+(n-1)k)(K-k)}\\ V_{\text{int}}&=\frac{1}{2}V_0 n(n-1)\sqrt{\frac{K-k}{K-k+\beta}}.\end{aligned} \tag{26}$$

K and k are to be determined from the minimizing of $\langle\mathbf{H}\rangle$. It is thus possible to represent the expected energy as function of the strength of the interaction (given by V_0) and the range of the interaction (given by $1/\beta$).

If there is no interaction we get $k=0$ and $K=2m\omega/\hbar$.

As a measure of the deviation of the wave function (25) from the corresponding independent particle wave function we take the correlation coefficient

$$\varrho=\frac{\langle \mathbf{x}_1\mathbf{x}_2\rangle}{\sqrt{\langle \mathbf{x}_1^2\rangle\langle \mathbf{x}_2^2\rangle}}. \tag{27}$$

which may be expressed as a function of K and k

$$\varrho=-\frac{(n-1)k}{K+(n-2)k}=-\frac{(n-1)(k_{\oplus}-k_{\ominus})}{(2n-3)(k_{\oplus}+k_{\ominus})}. \tag{28}$$

From the definition (27) follows that $-1\leqslant\varrho\leqslant+1$. In an independent particle description $\varrho=0$. $|\varrho|=1$ means that $\mathbf{x}_1$ and $\mathbf{x}_2$ are linearly dependent.

The extension of the methods discussed in this paragraph to three dimensions is straightforward in the symmetric case but the antisymmetric case is more involved because it is difficult to find a suitable two-particle wave function from which the total wave function may be constructed. The requirement which is hard to satisfy is that for certain values of the variational parameters the wave function must describe independent particles. We hope to be able to return to this point.

APPENDIX 1

Two interacting particles in a common potential

The system consists of two identical particles with mass m and coordinates $\vec{\mathbf{q}}_1$ and $\vec{\mathbf{q}}_2$ in a common oscillator potential

$$\frac{m}{2}(\vec{q}\cdot\omega\cdot\omega\cdot\vec{q})=\frac{m}{2}(\omega_x^2q_x^2+\omega_y^2q_y^2+\omega_z^2q_z^2) \tag{A 1.1}$$

where

$$\omega=\omega_x\hat{x}\hat{x}+\omega_y\hat{y}\hat{y}+\omega_z\hat{z}\hat{z}.$$

The interaction between the particles is determined by a potential $V(\vec{\mathbf{q}}_1-\vec{\mathbf{q}}_2)$. The Hamiltonian $\mathbf{H}$ of the system is then

$$\mathbf{H}=(1/2m)(\vec{\mathbf{p}}_1^2+\vec{\mathbf{p}}_2^2)+(m/2)(\vec{\mathbf{q}}_1\cdot\omega\cdot\omega\cdot\vec{\mathbf{q}}_1+\vec{\mathbf{q}}_2\cdot\omega\cdot\omega\cdot\vec{\mathbf{q}}_2)+V(\vec{\mathbf{q}}_1-\vec{\mathbf{q}}_2). \tag{A 1.2}$$

We introduce the new variables $\vec{\mathbf{r}}_{\oplus}$ and $\vec{\mathbf{r}}_{\ominus}$ by the transformation

$$\begin{aligned}\vec{\mathbf{q}}_1&=(1/\sqrt{2})(\vec{\mathbf{r}}_{\oplus}+\vec{\mathbf{r}}_{\ominus})\\ \vec{\mathbf{q}}_2&=(1/\sqrt{2})(\vec{\mathbf{r}}_{\oplus}-\vec{\mathbf{r}}_{\ominus}).\end{aligned} \tag{A 1.3}$$

The Hamiltonian $\mathbf{H}$ can now be written

$$\mathbf{H}=\mathbf{H}_{\oplus}+\mathbf{H}_{\ominus}, \tag{A 1.4}$$

where

$$\begin{aligned} \mathbf{H}_{\oplus} &= (1/2\,m)\,\vec{\mathbf{p}}_{\oplus}^{2} + (m/2)\,\vec{\mathbf{r}}_{\oplus}\cdot\boldsymbol{\omega}\cdot\boldsymbol{\omega}\cdot\vec{\mathbf{r}}_{\oplus} \\ \mathbf{H}_{\ominus} &= (1/2\,m)\,\vec{\mathbf{p}}_{\ominus}^{2} + (m/2)\,\vec{\mathbf{r}}_{\ominus}\cdot\boldsymbol{\omega}\cdot\boldsymbol{\omega}\cdot\vec{\mathbf{r}}_{\ominus} + V\,(\sqrt{2}\,\vec{\mathbf{r}}_{\ominus}). \end{aligned} \tag{A 1.5}$$

The two-particle eigenvalue problem

$$\mathbf{H}\,|\,E\,\rangle = E\,|\,E\,\rangle \tag{A 1.6}$$

is replaced by the two one-particle eigenvalue problems

$$\left.\begin{aligned} \mathbf{H}_{\oplus}\,|\,E_{\oplus}\,\rangle &= E_{\oplus}\,|\,E_{\oplus}\,\rangle \\ \mathbf{H}_{\ominus}\,|\,E_{\ominus}\,\rangle &= E_{\ominus}\,|\,E_{\ominus}\,\rangle \end{aligned}\right. \quad E = E_{\oplus} + E_{\ominus}. \tag{A 1.7}$$

The state vector $|\,E_{\ominus}\,\rangle$ must have even or odd parity corresponding to symmetry or antisymmetry of the two-particle state $|\,E\,\rangle$.

We shall now assume that

$$\begin{aligned} \boldsymbol{\omega} &= \omega\,\mathbf{1} \\ V\,(\sqrt{2}\,\vec{r}) &= \alpha\,(r) + \beta\,(r)\,r^{2} + \gamma\,(r)\,r^{-2} \quad (r = |\,\vec{r}\,|). \end{aligned} \tag{A 1.8}$$

The operators (A 1.5) are now both invariant under rotations. For the radial part $f\,(r)$ of the wave function we obtain in the $\ominus$-case the differential equation

$$\begin{aligned} \Bigg\{ \frac{d^{2}}{d\,r^{2}} - [l\,(l+1) + (2\,m/\hbar^{2})\,\gamma\,(r)]\,r^{-2} - \left[\frac{m^{2}\,\omega^{2}}{\hbar^{2}} + \frac{2\,m\,\beta\,(r)}{\hbar^{2}}\right] r^{2} + \\ + (2\,m/\hbar^{2})\,(E_{\ominus} - \alpha\,(r))\Bigg\}\,f\,(r) = 0. \end{aligned} \tag{A 1.9}$$

In an interval where α, β and γ are constants this equation may be transformed into Whittaker's differential equation

$$\left\{\frac{d^{2}}{d\,x^{2}}, \; - (1/4) + k, \; x^{-1} + (1/4 - \mu^{2})\,x^{-2}\right\} W\,(x) = 0. \tag{A 1.10}$$

The transformation is

$$\begin{aligned} x &= \lambda\,r^{2} \\ W &= \sqrt{2\,\lambda}\,r\,f\,(r). \end{aligned} \tag{A 1.11}$$

The parameters in Whittaker's equation are determined from the relations

$$\begin{aligned} \lambda^{2} &= (m^{2}\,\omega^{2}/\hbar^{2}) + (2\,m\,\beta\,(r)/\hbar^{2}) \\ 4\,\mu^{2} - 1/4 &= l\,(l+1) + (2\,m\,\gamma\,(r)/\hbar^{2}) \\ 2\,\lambda\,k &= m\,(E_{\ominus} - \alpha\,(r))/\hbar^{2}. \end{aligned} \tag{A 1.12}$$

APPENDIX 2

Two interacting one-dimensional particles in a common potential. Variational treatment

The Hamiltonian for two one-dimensional particles, coordinates q_1 and q_2, with Gauszian interaction, in a common oscillator potential, is

$$\mathbf{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial q_1^2}+\frac{\partial^2}{\partial q_2^2}\right)+\frac{m\,\omega^2}{2}(q_1^2+q_2^2)-V_0 e^{-\frac{1}{4}\left(\frac{q_1-q_2}{\theta}\right)^2}. \tag{A 2.1}$$

Introducing

$$\begin{aligned} x_1 &= (1/\sqrt{2})\,(q_1+q_2) \\ x_2 &= (1/\sqrt{2})\,(q_1-q_2), \end{aligned} \tag{A 2.2}$$

we get

$$\mathbf{H} = -\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x_1^2}+\frac{\partial^2}{\partial x_2^2}\right)+\frac{m\,\omega^2}{2}(x_1^2+x_2^2)-V_0 e^{-\frac{1}{2}\left(\frac{x_2}{\theta}\right)^2}\equiv$$

$$\equiv \mathbf{H}_1\left(x_1,\frac{\partial}{\partial x_1}\right)+\mathbf{H}_2\left(x_2,\frac{\partial}{\partial x_2}\right). \tag{A 2.3}$$

The orthonormalized eigenfunctions $\phi_n(x)$ of the operator

$$\mathbf{\Omega} = -\frac{\partial^2}{\partial x^2}+\frac{1}{4}x^2 \tag{A 2.4}$$

are

$$\phi_n(x) = (1/2\pi)^{\frac{1}{4}}(1/n!)^{\frac{1}{2}}\left[-\frac{\partial}{\partial x}+\frac{1}{2}x\right]^n e^{-\frac{1}{4}x^2} =$$

$$= (1/2\pi)^{\frac{1}{4}}(1/n!)^{\frac{1}{2}}\left(-\frac{\partial}{\partial x}\right)^n e^{-\frac{1}{2}x^2}. \tag{A 2.5}$$

The y satisfy the equations

$$\mathbf{\Omega}\,\phi_n(x) = (n+1/2)\,\phi_n(x). \tag{A 2.6}$$

If

$$\Delta^2 = (\hbar/2\,m\,\omega) \tag{A 2.7}$$

the n:th eigenfunction of a harmonic oscillator with mass m and frequency ω is

$$(1/\Delta)^{\frac{1}{2}}\phi_n(x/\Delta). \tag{A 2.8}$$

We approximate the eigenfunctions of the operator $H_2\left(x,\frac{\partial}{\partial x}\right)$ by oscillator wave functions obtained from the minimizing of the expression

$$F_n(\sigma^2) = \int_{-\infty}^{+\infty}\phi_n(x/\sigma)\,H_2\left(x,\frac{\partial}{\partial x}\right)\phi_n(x/\sigma)\,dx/\sigma \tag{A 2.9}$$

over σ^2. According to the definition (A 2.5)

$$\frac{\partial^2}{\partial x^2}\,\phi_n\left(\frac{x}{\sigma}\right)=\frac{1}{\sigma^2}\left\{\frac{1}{4}\left(\frac{x}{\sigma}\right)^2-(n+1/2)\right\}\phi_n\left(\frac{x}{\sigma}\right).$$

We introduce the notations

$$a_n=\int_{-\infty}^{+\infty}|\,\phi_n(x)\,|^2\,x^2\,d\,x \tag{A 2.10}$$

$$b_n(\alpha)=\int_{-\infty}^{+\infty}|\,\phi_n(x)\,|^2\,e^{-\frac{1}{2}\alpha x^2}\,d\,x, \tag{A 2.11}$$

and obtain for $F_n(\sigma^2)$

$$F_n(\sigma^2)=-\frac{\hbar^2}{2\,m\,\sigma^2}\left\{\frac{a_n}{4}-(n+1/2)+\frac{m\,\omega^2\,\sigma^2}{2}\,a_n-V_0\,b_n\left(\left(\frac{\sigma}{\theta}\right)^2\right)\right\}. \tag{A 2.12}$$

For the determination of a_n and $b_n(\alpha)$ we use the identity

$$\sum_0^{\infty}|\,\phi_n(x)\,|^2\,t^n=(1/2\,\pi)^{\frac{1}{2}}\,(1/(1-t^2))^{\frac{1}{2}}\,e^{-\frac{1}{2}x^2(1-t/1+t)} \tag{A 2.13}$$

If both sides are multiplied by x^2 and by $e^{-\frac{1}{2}\alpha x^2}$ respectively and the equality then integrated over x we get

$$\sum_{n=0}^{\infty}t^n\int_{-\infty}^{\infty}|\,\phi_n(x)\,|^2\,x^2\,d\,x=\sum_{n=0}^{\infty}a_n\,t^n=(1+t/(1-t)^2) \tag{A 2.14}$$

and

$$\sum_{n=0}^{\infty}t^n\int_{-\infty}^{+\infty}|\,\phi_n(x)\,|^2\,e^{-\frac{1}{2}\alpha x^2}\,d\,x=\sum_{n=0}^{\infty}b_n(\alpha)\,t^n=((1-\alpha)\,t^2-2\,t+1+\alpha)^{-\frac{1}{2}} \tag{A 2.15}$$

From (A 2.14 and 15) we obtain a_n and $b_n(\alpha)$ by derivation with respect to t n times and then putting $t=0$. The first few coefficients are

$$\begin{array}{ll}
a_0=1 & b_0(\alpha)=(1+\alpha)^{-\frac{1}{2}}\\
a_1=3 & b_1(\alpha)=(1+\alpha)^{-\frac{3}{2}}\\
a_2=5 & b_2(\alpha)=-\frac{1}{2}(1-\alpha)(1+\alpha)^{-\frac{3}{2}}+(3/2)(1+\alpha)^{-\frac{5}{2}}\\
\ldots & \\
a_n=2\,n+1 &
\end{array} \tag{A 2.16}$$

Finally we obtain for $F_n(\sigma^2)$

$$F_n(\sigma^2)=\hbar\,\omega\left\{\frac{2\,n+1}{4}\left(\xi+\frac{1}{\xi}\right)-v_0\,b_n\left(\xi\left(\frac{\Delta}{\theta}\right)^2\right)\right\}.$$

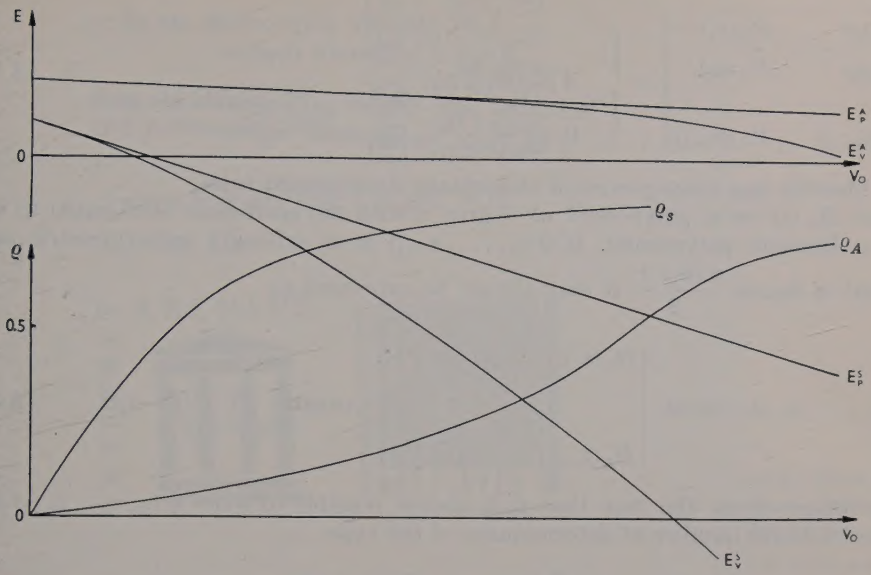

Fig. 1. Dependence of the energy E of two interacting particles in a common oscillator potential on the strength of the interaction V_0. Range of the interaction $\theta = \sqrt{\hbar/20\, m\, \omega}$.

E^A_V ground state energy for fermions (variational method);
E^A_P ground state energy for fermions (first order perturbation theory);
E^S_V ground state energy for bosons (variational method);
E^S_P ground state energy for bosons (first order perturbation theory).

The statistical dependence of the coordinates of the particles is represented by the correlation coefficient ϱ as a function of V_0 (see (27) and (28)).

where

$$\xi = \frac{\sigma^2}{\Delta^2} \quad \text{and} \quad V_0 = \hbar\, \omega\, v_0.$$

It should be remarked that $\Delta^2 = (\hbar/2\, m\, \omega)$ is the standard deviation of the coordinate of an oscillator in its groundstate, and $a_n\, \Delta^2$ is the standard deviation in the n:th excited state. θ may be called the range of the two-particle interaction.

It is now possible to calculate the energy of the two-particle system as a function of the range (θ) and strength ($V_0 = \hbar\, \omega\, v_0$) of the interaction. The result of such a calculation is shown in figure 1, and a comparison with ordinary first order perturbation theory is made.

APPENDIX 3

If $P_0(z), P_1(z), \ldots, P_n(z)$ are $n+1$ polynomials with degree not higher than n, and if the coefficient of the highest power of z is one in each polynomial, the following identity holds

$$\begin{vmatrix} P_0(z_1) & \dots P_n(z_1) \\ P_0(z_2) & \dots P_n(z_2) \\ \cdot\ \cdot\ \cdot & \cdot\ \cdot\ \cdot \\ P_0(z_{n+1}) & \dots P_n(z_{n+1}) \end{vmatrix} = \begin{cases} \prod\limits_{1\leqslant i<j\leqslant n+1} (z_i - z_j) & \text{if the polynomials are of different degrees} \\ 0 & \text{if two polynomials are of the same degree} \end{cases} \tag{A 3.1}$$

The identity is a consequence of elementary determinant rules.

Let $H_n(z)$ be a polynomial of degree n with the coefficient of z^n equal to one, e.g. a Hermite polynomial. If $Q(z_1, \dots, z_{n+1})$ is an arbitrary antisymmetric polynomial of degree $\frac{n(n+1)}{2}$ it may always be expressed as

$$Q(z_1, \dots, z_{n+1}) = \text{const.} \begin{vmatrix} H_0(z_1) & \dots H_n(z_1) \\ \cdot\ \cdot\ \cdot & \cdot\ \cdot\ \cdot \\ \cdot\ \cdot\ \cdot & \cdot\ \cdot\ \cdot \\ H_0(z_{n+1}) & \dots H_n(z_{n+1}) \end{vmatrix} = \text{const.} \prod_{1\leqslant i<j\leqslant n+1} (z_i - z_j). \tag{A 3.2}$$

This follows from the fact that it is always possible to write $Q(z_1, \dots, z_{n+1})$ as a sum of a finite number of determinants of the type

$$\begin{vmatrix} H_{i0}(z_1) & \dots H_{in}(z_1) \\ \cdot\ \cdot\ \cdot & \cdot\ \cdot\ \cdot \\ H_{i0}(z_{n+1}) & \dots H_{in}(z_{n+1}) \end{vmatrix}$$

with constant coefficients. According to (A 3.1) the only nonvanishing determinant of this type is (A 3.2).

The present investigation was carried out at the Institute of Theoretical Physics in Stockholm, and we wish to express our sincere gratitude to Professor O. Klein, Director of the institute, for his kind interest in our work. We are indebted to the Swedish Atomic Committee for financial support.

Institute of Theoretical Physics, Stockholm, October 1957.

REFERENCES

1. Brueckner, K. A., and Levinson, C. A., Phys. Rev. *97* (1955) 1344; also Bethe, H. A., Phys. Rev. *103*, 1353 (1956) where an extensive list of references to other work of Brueckner and coll. can be found.
2. Hugenholtz, N. M., Physica *23*, 533 (1957).
3. Jastrow, R., Phys. Rev. *98*, 1479 (1955). Dyson, F. J., Phys. Rev. *106*, 20 (1957).

Tryckt den 13 februari 1958

Uppsala 1958. Almqvist & Wiksells Boktryckeri AB